

Interstellar Grains: Effect of Inclusions on Extinction

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A composite dust grain model which simultaneously explains the observed interstellar extinction, polarization, IR emission and the abundance constraints, is required. We present a composite grain model, which is made up of a host silicate oblate spheroid and graphite inclusions. The interstellar extinction curve is evaluated in the spectral region $3.4\text{--}0.1\mu\text{m}$ using the extinction efficiencies of the composite spheroidal grains for three axial ratios. Extinction curves are computed using the discrete dipole approximation (DDA). The model curves are subsequently compared with the average observed interstellar extinction curve and with an extinction curve derived from the IUE catalogue data.

Key words: Interstellar Dust, Extinction

1. Introduction

It is highly unlikely that the interstellar grains are spherical in shape or that they are homogeneous in composition and structure. The collected interplanetary particles are nonspherical and highly porous and composites of very small sub-grains glued together (Brownlee, 1987). The existence of interstellar polarization requires that the interstellar grains must be nonspherical. The elemental abundances derived from the observed interstellar extinction also do not favour the homogeneous composition for the interstellar grains. There is no exact theory to study light scattering by inhomogeneous grains

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(viz. porous, fluffy and composite). We have used Discrete Dipole Approximation (DDA) to study the extinction properties of the composite grains. For the description on the DDA see Draine (1988). In the present study, we calculate the extinction efficiencies for the composite oblate spheroidal grains, made up of the host silicate spheroid with embedded inclusions of graphite, in the wavelength region, 3.4-0.10 μm . Using these extinction efficiencies of the composite grains with a power law grain size distribution we evaluate the interstellar extinction curve. We also estimate the cosmic abundances viz. silicon and carbon for the grain models which fit the observed interstellar extinction curve. It must be mentioned here that the composite oblate grain model presented in this study has also been used to interpret the observed IR emission from circumstellar dust (Vaidya & Gupta, 2011).

In section 2 we give the validity criteria for the DDA and the composite oblate grain models. In section 3 we present the results of our computations and discuss them. The main conclusions of our study are given in section 4.

1.1 Composite grains and DDA

In the Discrete Dipole Approximation (DDA), a solid particle is replaced (approximated) by an array of N dipoles. When a grain is exposed to an electromagnetic wave, each dipole responds to the radiation field of the incident wave as well as to the fields of the other $N-1$ dipoles that comprise the grain (Draine, 1988).

We use the computer code developed by Dobbie (see Vaidya et. al., 2001) to generate the composite oblate grain models used in the present study. The constituent materials of the composite grains consist of silicates and graphites, since in the interstellar medium, carbon and silicate occur separately and in the form of small particles which are agglomerated into large grains. For detailed discussion on the composition of the composite interstellar dust see Mathis (1996) and Vaidya et. al. (2001). We have studied composite grain models with a host silicate spheroid containing $N= 9640, 25896$ and 14440 dipoles, each carved out from $32 \times 24 \times 24, 48 \times 32 \times 32$ and $48 \times 24 \times 24$ dipole sites, respectively; sites outside the spheroid are set to be vacuum and sites inside are assigned to be the host material. It is to be

noted that the composite oblate spheroidal grain with $N=9640$ has an axial ratio (AR) of 1.33, whereas $N=25896$ has the axial ratio of 1.5 and $N=14440$ has the axial ratio of 2.0. Further, if the semi-major axis and semi-minor axis are denoted by $x/2$ and $y/2$, respectively, then $a^3 = (x/2)(y/2)^2$, where a is the radius of the sphere whose volume is same as of a spheroid. To study randomly oriented spheroids, it is necessary to get the scattering properties of the composite grains over all possible orientations. We use three values of each of the orientation parameters (β, θ and ϕ). i.e. averaging over 27 orientations, which we find is quite adequate (see Wolf et al., 1994). The volume fractions of the graphite inclusions used are 10%, 20% and 30% (denoted as $f=0.1, 0.2$ and 0.3). The size of the inclusion is given by the number of dipoles, 'n' across the diameter of an inclusion; e.g. 152 for composite grain model with $N=9640$ i.e. $AR=1.33$ (see Table I in Vaidya and Gupta, 2011). Details on the computer code and the corresponding modification to the DDSCAT 6.1 code (Draine & Flatau 2003) are given in Vaidya et al. (2001) and Gupta et al. (2006). The modified code outputs a three-dimensional matrix specifying the material type at each dipole site; the sites are either silicate, graphite or vacuum. For an illustrative example of a composite oblate spheroidal grain with $N=14440$ dipoles ($AR=2.00$), please refer Figure 1, given in Gupta et al. (2006). There are two validity criteria for DDA (see e.g. Wolff et al. 1994); viz. (i) $|m|kd \leq 1$, where m is the complex refractive index of the material, $k=\pi/\lambda$ is the wavenumber and d is the lattice dispersion spacing and (ii) d should be small enough (N should be sufficiently large) to describe the shape of the particle satisfactorily. The complex refractive indices for silicates and graphite are obtained from Draine (1985, 1987). For all the composite grain models, with $N=9640, 25896$ and 14440 (i.e. $AR=1.33, 1.50$ & 2.00 respectively) and for all the grain sizes, between $a = 0.001-0.250\mu$, in the wavelength range of $3.4-0.1\mu m$, considered in the present study; we have checked that the DDA criteria are satisfied (Vaidya et al. 2007).

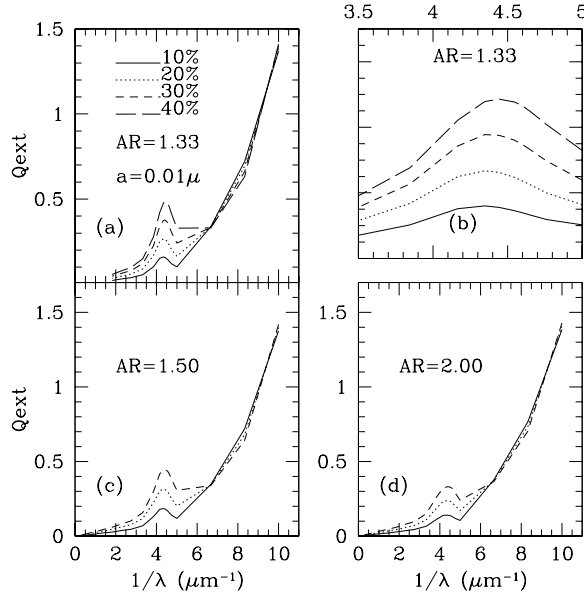


Fig. 1. Extinction Efficiencies for the composite grains of size 0.01μ with host spheroids containing dipoles $N=9640$, 25896 and 14440 ; corresponding to the axial ratio 1.33 , 1.50 and 2.00 respectively, are shown in (a),(c) and (d) in the wavelength region, $3.4-0.10\mu m$ for three graphite inclusion fractions ($f=0.1$, 0.2 and 0.3 corresponding to 10% , 20% and 30% inclusion fractions). An additional 40% inclusion case for $AR=1.33$ ($N=9640$) is shown in the panels (a) and (b). In panel (b) the extinction curves in the wavelength region $0.28-0.20\mu m$ are highlighted.

2. Results

2.1 Extinction Efficiency of Composite Grains

In the present paper, we study the extinction properties of the spheroidal grains with three axial ratios (AR), viz. 1.33 , 1.5 and 2.0 , corresponding to the grain models with $N=9640$, 25896 and 14440 respectively, for three volume fractions of inclusions; viz. 10% , 20% and 30% , in the wavelength region $3.4-0.10\mu m$. Figures 1 (a),(c) and (d) show the extinction efficiencies (Q_{ext}) for the composite grains with the host silicate spheroids containing $N=9640$, 25896 and 14440 dipoles, corresponding to axial ratio 1.33 , 1.5 and 2.0 respectively with a host composite grain size set to $a=0.01\mu$. The three volume fractions, viz. 10% , 20% and 30% , of graphite inclusions are also listed in the top (a) panel and an additional volume fraction of 40% is also displayed. The extinction in the spectral region $0.28-0.20\mu m$ is highlighted in the panel (b) of this figure for the composite grains with $N=9640$.

The effect of the variation of volume fraction of inclusions is clearly seen for all the models. The extinction efficiency increases as the volume fraction of the graphite inclusion increases. It is to be

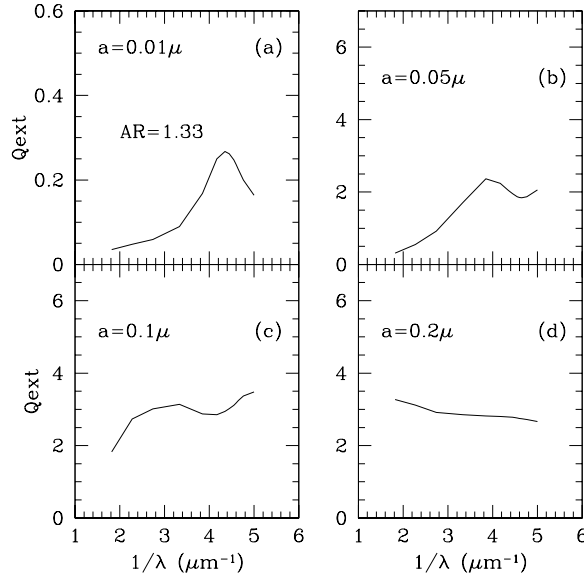


Fig. 2. Extinction efficiencies for the composite grains with AR=1.33 (N=9640) and with 20% volume fraction of graphite inclusions for various grain sizes.

noted that the wavelength of the peak extinction shifts with the variation in the volume fraction of inclusions. These extinction curves also show the variation in the width of the extinction feature with the volume fraction of inclusions. All these results indicate that the inhomogeneities within the grains play an important role in modifying the '2175Å' feature. Voshchinnikov (1990) and Gupta et al. (2005) had found variation in the '2175Å' feature with the shape of the grain, and Iati et al. (2001, 2004); Voshchinnikov (2002); Voshchinnikov and Farafanov (1993) and Vaidya et al. (1997, 1999) had found the variation in the feature with the porosity of the grains. Draine & Malhotra (1993) have found relatively little effect on either the central wavelength or the width of the feature for the coagulated graphite silicate grains. Figures 2(a-d) show the extinction efficiencies (Q_{ext}) for the composite grains for four host grain sizes: viz. $a=0.01$, 0.05 , 0.1 and 0.2μ at a constant volume fraction of inclusion of 20%. It is seen that the extinction and the shape of the extinction curves varies considerably as the grain size increases. The '2175Å feature' is clearly seen for small grains; viz. $a=0.01$ and 0.05μ , whereas for larger grains the feature almost disappears.

2.2 Interstellar Extinction Curve

The interstellar extinction curve (i.e. the variation of extinction with wavelength) is usually expressed by the ratio $E(\lambda - V)/E(B - V)$ versus $1/\lambda$. We use the extinction efficiencies of the composite grains, with a power law size distribution (i.e. $n(a) \sim a^{-3.5}$, (Mathis et. al 1977) to evaluate the interstellar extinction curve in the wavelength region of $3.4-0.10\mu m$. In addition to the composite grains, a separate component of small graphite grains is required to produce the observed peak at 2175\AA in the interstellar extinction curve (Mathis, 1996). The stability of the bump at 2175\AA along all the lines of sight rules out the possibility of using just composite grains, made up of silicate with graphite as inclusions, to produce the bump (Iati et al. 2001).

The average observed interstellar extinction curve (Whittet, 2003) is then compared with the model curves formed from a χ^2 minimized and best fit linear combination of the composite and graphite grains (for details see Vaidya & Gupta 1999).

Figure 3(a) shows the interstellar extinction curve for the composite grains with $AR=1.33$ ($N=9640$) in the entire wavelength region of $3.4 - 0.10\mu m$ for the MRN grain size distribution, with the size range, $a=0.005-0.250\mu$. It is seen that the composite spheroidal grain models with $AR=1.33$ ($N=9640$) and $f=0.1$ fits the average observed extinction curve reasonably well in the wavelength range considered, i.e $3.4 - 0.10\mu m$. The model extinction curves with $AR=1.50$ & 2.00 ($N=25896$ & 14440 respectively) deviate from the observed extinction curve in the uv region, beyond the wavelength $\sim 0.1500\mu m$ (i.e. $6\mu m^{-1}$) and are thus not shown in the figure. These results with the composite grains indicate that the spheroidal grains with the axial ratio not very large i.e $AR \sim 1.33$ ($N=9640$) is an optimum choice. The results indicate that a third component of very small grains (e.g very small silicate grains or PAHs) may be required to explain the extinction beyond 1500\AA in the UV (Weingartner and Draine, 2001).

In the Figure 3(b), we have displayed the observed extinction curve in the direction of the star HD46202 (data taken from IUE data base) and its best fitting with the model $AR=1.50$ ($N=25896$) and grain size distribution of $a=0.001-0.100\mu$. We have selected this particular star with $R_v = 3.1$,

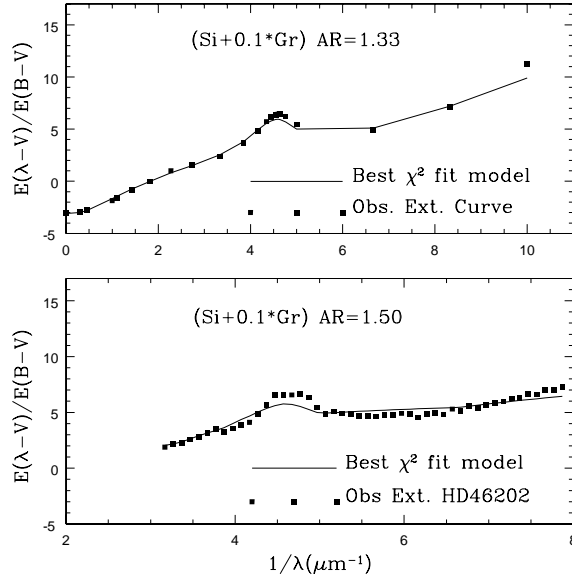


Fig. 3. (a) Comparison of the observed interstellar extinction curve (Whittet, 2003) with the best fit model curve of composite grains with graphite inclusions in the wavelength range of $3.4\text{--}0.1\mu\text{m}$. (b) Observed Extinction curve in the direction of the star HD46202 and its comparison with model curve of AR=1.50.

from our recent analysis of extinction curves towards the directions of 48 IUE stars (Katy al, al., 2011)

Recently Iati et. al. (2004), Zubko et. al (2004) Voshchinnikov et. al. (2005) and Maron & Maron (2005) have also proposed composite grain models. Very recently Voshchinnikov et. al (2006) have proposed composite porous grain models with three or more grain populations and have used both EMT-Mie type and layered sphere calculations.

2.3 Cosmic Abundances

In addition to reproducing the interstellar extinction curve, any grain model must also be consistent with the abundance constraints. Snow and Witt (1995, 1996) have reviewed several models for the interstellar dust, which provide the data on the quantities of some elements that are required to reproduce the interstellar extinction. The number of atoms (in ppm) of the particular material tied up in grains can be estimated if the atomic mass of the element in the grain material and the density of the material are known (see e.g. Cecchi-Pestellini et al. 1995 and Iati et al. 2001). From the composite grain models we have proposed, we estimate C abundance i.e. C/H between $\sim 165\text{--}200$

(including those atoms that produce the 2175\AA feature), which is considerably lower than what is predicted by bare silicate/graphite grain models (e.g. $\text{C/H} \sim 254$ ppm, Li and Draine, 2001) but it is still significantly above the ISM value of ~ 110 (Mathis 2000); ~ 140 (Sofia & Meyer, 2001) and ~ 100 (Sofia & Parvathy, 2009). The estimated Si abundance from the composite grain model presented here is between 25 and 30, which is lower than the other grain models, 32 ppm (Li and Draine, 2001) and is consistent with the recent ISM value of 25 ppm derived by Voshchinnikov & Henning (2010). For appropriate reference on abundance standards and related topics see Snow (2000) and Draine (2003).

3. Summary and Conclusions

Using the discrete dipole approximation (DDA) we have studied the extinction properties of the composite spheroidal grains, made up of the host silicate and graphite inclusions in the wavelength region of $3.4\text{--}0.10\mu\text{m}$. Our main conclusions from this study are:

(1) The extinction curves for the composite spheroidal grains show a shift in the central wavelength of the extinction peak as well as variation in the width of the peak with the variation in the volume fraction of the graphite inclusions. These results clearly indicate that the shape, structure and inhomogeneity in the grains play an important role in producing the extinction. It must be noted here that large PAH molecules are also candidates to the carrier of the interstellar 2175\AA feature – a natural extension of the graphite hypothesis (Draine, 2003).

(2) The extinction curves for the composite spheroidal grains with the axial ratio not very large ($\text{AR} \sim 1.33$, $N=9640$) and 10 % volume fractions of graphite inclusions are found to fit the average observed interstellar extinction satisfactorily. Extinction curves with other composite grain models with $N=25896$ and 14440 (i.e. with axial ratios of 1.50 and 2.00) deviate from the observed curves in the UV region, i.e. beyond about wavelength 1500\AA . These results indicate that a third component of very small particles in the composite grains may help improve the fit in the UV region (see e.g. Weingartner and Draine 2001). It must be mentioned here that the composite spheroidal grain model with silicate

and graphite as constituent materials proposed by us is not unique (see e.g. Zubko et al., 2004). We have also attempted to fit models to a specific direction of the star HD46202 in our galaxy and show that $AR=1.50$ ($N=25896$) fits better in this case. Analysis is in progress for many more such directions in the galaxy.

(3) These results clearly show that composite grain model is more efficient, compared to bare silicate/graphite grain models, in producing the extinction and it would perhaps help reducing the cosmic abundance constraints. Composite grain models with silicate, graphite and an additional component (e.g. PAH's) may further reduce the abundance constraints.

We have used the composite spheroidal grain model to fit the observed interstellar extinction and have derived the abundance of carbon (C/H) and silicon (Si/H). The IRAS observations have indicated the importance of the IR emission as a constraint on interstellar dust models (Zubko et al. 2004). Recently, we have used the composite spheroidal grain model to fit the IR emission curves obtained from IRAS observations (Vaidya & Gupta, 2011).

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